

Acetic acid, (hexyloxy)-
57931-25-6 | DTXSID9069211

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 1.72e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.84e-01

Confidence level: 7.29e-01

Nearest Neighbors from the Training Set

Image not found

(Cyclopentyloxy)acetic acid

Measured: 1.42e-01

Predicted: 1.96e-01

Image not found

Propionic acid, 2-(cyclohexyloxy)-2-methyl-

Measured: 8.32e-02

Predicted: 6.22e-02

Image not found

4-Ethoxy-3-methyl-4-oxobut-2-enoate

Measured: 9.42e-02

Predicted: 1.51e-01